

On the k -independence number of graphs

A. Abiad^{a,b}, G. Coutinho^c, M. A. Fiol^d

^aDepartment of Quantitative Economics

Maastricht University, Maastricht, The Netherlands,

^bDepartment of Mathematics: Analysis, Logic and Discrete Mathematics

Ghent University, Ghent, Belgium,

a.abiadmonge@maastrichtuniversity.nl

^cDepartment of Computer Science

Federal University of Minas Gerais, Belo Horizonte, Brazil

gmcout@gmail.com

^dDepartament de Matemàtiques

Universitat Politècnica de Catalunya, Barcelona, Catalonia

Barcelona Graduate School of Mathematics

miguel.angel.fiol@upc.edu

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Abstract

This paper generalizes and unifies the existing spectral bounds on the k -independence number of a graph, which is the maximum size of a set of vertices at pairwise distance greater than k . The previous bounds known in the literature follow as a corollary of the main results in this work. We show that for most cases our bounds outperform the previous known bounds. Some infinite families of graphs where the bounds are tight are also presented. Finally, as a byproduct, we derive some spectral lower bounds for the diameter of a graph.

Keywords: Graph, k -independence number, Spectrum, Interlacing, Regular partition, Antipodal distance-regular graph, Diameter.

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1 Introduction

Given a graph G , let $\alpha_k = \alpha_k(G)$ denote the size of the largest set of vertices such that any two vertices in the set are at distance larger than k . This choice of notation is no

coincidence, since actually α_1 is just the independence number of a graph. The parameter $\alpha_k(G)$ therefore represents the largest number of vertices which can be $k + 1$ spread out in G . It is known that determining α_k is NP-Hard in general [19].

The k -independence number of a graph is directly related to other combinatorial parameters such as the average distance [13], packing chromatic number [14], injective chromatic number [18], and strong chromatic index [21]. Upper bounds on the k -independence number directly give lower bounds on the corresponding distance or packing chromatic number. Regarding it, Alon and Mohar [2] asked for the extremal value of the distance chromatic number for graphs of a given girth and degree.

In this paper we generalize and improve the known spectral upper bounds for the k -independence number from [8] and [1]. For some cases, we also show that our bounds are sharp.

As far as we are aware, there seems to be some conflict in the existing literature regarding the use of the term ‘ k -independence number’. The following list contains the three conflicting definitions, which all, nonetheless, are a natural generalization of the concept of independence number.

1. Caro and Hansberg [6] use the term ‘ k -independence number’ to denote the maximum size of a set of vertices in a graph whose induced subgraph has maximum degree k . Thus, α_0 is the usual independence number.
2. Špacapan [22] uses ‘ k -independence number’ to denote the size of the largest k -colourable subgraph of G . With this notation, α_1 stands for the usual independence number of G .
3. Fiol [8] and Abiad, Tait, and Cioabă [1] use ‘ k -independence number’ to denote the size of the largest set of vertices such that any two vertices in the set are at distance larger than k .

The latter definition is the one we use in this work.

The first known spectral bound for the independence number α is due to Cvetković [7].

Theorem 1.1 (Cvetković [7]). *Let G be a graph with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. Then,*

$$\alpha \leq \min\{|\{i : \lambda_i \geq 0\}| \quad \text{and} \quad |\{i : \lambda_i \leq 0\}|\}.$$

Another well-known result is the following bound due to Hoffman (unpublished; see for instance Haemers [16]).

Theorem 1.2 (Hoffman [16]). *If G is a regular graph on n vertices with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$, then*

$$\alpha \leq n \frac{-\lambda_n}{\lambda_1 - \lambda_n}.$$

Regarding the k -independence number, the following three results are known. The first is due to Fiol [8] and requires a preliminary definition. Let G be a graph with distinct eigenvalues $\theta_0 > \dots > \theta_d$. Let $P_k(x)$ be chosen among all polynomials $p(x) \in \mathbb{R}_k(x)$, that is, polynomials of real coefficients and degree at most k , satisfying $|p(\theta_i)| \leq 1$ for all $i = 1, \dots, d$, and such that $P_k(\theta_0)$ is maximized. The polynomial $P_k(x)$ defined above is called the k -alternating polynomial of G and was shown to be unique in [11], where it was used to study the relationship between the spectrum of a graph and its diameter.

Theorem 1.3 (Fiol [8]). *Let G be a d -regular graph on n vertices, with distinct eigenvalues $\theta_0 > \dots > \theta_d$ and let $P_k(x)$ be its k -alternating polynomial. Then,*

$$\alpha_k \leq \frac{2n}{P_k(\theta_0) + 1}.$$

The second and third bounds are due to Abiad, Cioabă, and Tait [1]. The first is a Cvetković-like approach, whereas the second resembles Hoffman's.

Theorem 1.4 (Abiad, Cioabă, Tait [1]). *Let G be a graph on n vertices with adjacency matrix \mathbf{A} , with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. Let w_k and W_k be respectively the smallest and the largest diagonal entries of \mathbf{A}^k . Then,*

$$\alpha_k \leq |\{i : \lambda_i^k \geq w_k(G)\}| \quad \text{and} \quad \alpha_k \leq |\{i : \lambda_i^k \leq W_k(G)\}|.$$

Theorem 1.5 (Abiad, Cioabă, Tait [1]). *Let G be a δ -regular graph on n vertices with adjacency matrix \mathbf{A} , whose distinct eigenvalues are $\theta_0 (= \delta) > \dots > \theta_d$. Let \widetilde{W}_k be the largest diagonal entry of $\mathbf{A} + \mathbf{A}^2 + \dots + \mathbf{A}^k$. Let $\theta = \max\{|\theta_1|, |\theta_d|\}$. Then,*

$$\alpha_k \leq n \frac{\widetilde{W}_k + \sum_{j=1}^k \theta^j}{\sum_{j=1}^k \delta^j + \sum_{j=1}^k \theta^j}.$$

2 Preliminaries

For basic notation and results see [3, 15]. Let $G = (V, E)$ be a graph with $n = |V|$ vertices, $m = |E|$ edges, and adjacency matrix \mathbf{A} with spectrum $\text{sp } G = \{\theta_0 > \theta_1^{(m_1)} > \dots > \theta_d^{(m_d)}\}$, where the superscripts denote multiplicities. When the eigenvalues are presented with possible repetitions, we shall indicate them by $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Let us consider the scalar product in $\mathbb{R}_d[x]$:

$$\langle f, g \rangle_G = \frac{1}{n} \text{tr}(f(\mathbf{A})g(\mathbf{A})) = \frac{1}{n} \sum_{i=0}^d m_i f(\theta_i) g(\theta_i).$$

The so-called *predistance polynomials* $p_0 (= 1), p_1, \dots, p_d$ are a sequence of orthogonal polynomials with respect to the above product, with $\text{dgr } p_i = i$, and are normalized in

such a way that $\|p_i\|_G^2 = p_i(\theta_0)$ (this makes sense since it is known that $p_i(\theta_0) > 0$) for $i = 0, \dots, d$. Therefore they are uniquely determined, for instance, following the Gram-Schmidt process. They were introduced by Fiol and Garriga in [10] to prove the so-called ‘spectral excess theorem’ for distance-regular graphs. We also use the sum polynomials $q_i = p_0 + \dots + p_i$, for $i = 0, \dots, d-1$, which are also a sequence of orthogonal polynomials, now with respect to the scalar product

$$\langle f, g \rangle_{[G]} = \frac{1}{n} \sum_{i=0}^{d-1} m_i (\theta_0 - \theta_i) f(\theta_i) g(\theta_i),$$

(see [12, Prop. 4.3] for a proof) and satisfy $1 = q_0(\theta_0) < q_1(\theta_0) < \dots < q_{d-1}(\theta_0) < n$. See [5] for further details and applications.

Eigenvalue interlacing is a powerful and old technique that has found countless applications in combinatorics and other fields. This technique will be used in several of our proofs. For more details, historical remarks and other applications see Fiol and Haemers [9, 16].

Given square matrices \mathbf{A} and \mathbf{B} with respective eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ and $\mu_1 \geq \dots \geq \mu_m$, with $m < n$, we say that the second sequence *interlaces* the first if, for all $i = 1, \dots, m$, it follows that

$$\lambda_i \geq \mu_i \geq \lambda_{n-m+i}.$$

Theorem 2.1 (Interlacing [9, 16]). *Let \mathbf{S} be a real $n \times m$ matrix such that $\mathbf{S}^T \mathbf{S} = \mathbf{I}$, and let \mathbf{A} be a $n \times n$ matrix with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. Define $\mathbf{B} = \mathbf{S}^T \mathbf{A} \mathbf{S}$, and call its eigenvalues $\mu_1 \geq \dots \geq \mu_m$. Then,*

- (i) *The eigenvalues of \mathbf{B} interlace those of \mathbf{A} .*
- (ii) *If $\mu_i = \lambda_i$ or $\mu_i = \lambda_{n-m+i}$, then there is an eigenvector \mathbf{v} of \mathbf{B} for μ_i such that $\mathbf{S}\mathbf{v}$ is eigenvector of \mathbf{A} for μ_i .*
- (iii) *If there is an integer $k \in \{0, \dots, m\}$ such that $\lambda_i = \mu_i$ for $1 \leq i \leq k$, and $\mu_i = \lambda_{n-m+i}$ for $k+1 \leq i \leq m$ (tight interlacing), then $\mathbf{S}\mathbf{B} = \mathbf{A}\mathbf{S}$.*

Two interesting particular cases where interlacing occurs (obtained by choosing appropriately the matrix \mathbf{S}) are the following. Let \mathbf{A} be the adjacency matrix of a graph $G = (V, E)$. First, if \mathbf{B} is a principal submatrix of \mathbf{A} , then \mathbf{B} corresponds to the adjacency matrix of an induced subgraph G' of G . Second, when, for a given partition of the vertices of Γ , say $V = U_1 \cup \dots \cup U_m$, \mathbf{B} is the so-called *quotient matrix* of \mathbf{A} , with elements b_{ij} , $i, j = 1, \dots, m$, being the average row sums of the corresponding block \mathbf{A}_{ij} of \mathbf{A} . Actually, the quotient matrix \mathbf{B} does not need to be symmetric or equal to $\mathbf{S}^T \mathbf{A} \mathbf{S}$, but in this case \mathbf{B} is similar to—and therefore has the same spectrum as— $\mathbf{S}^T \mathbf{A} \mathbf{S}$. In the second case, if the interlacing is tight, Theorem 2.1(iii) reflects that \mathbf{S} corresponds to a *regular* (or *equitable*) partition of \mathbf{A} , that is, each block of the partition has constant row and column

sums. Then, the bipartite induced subgraphs G_{ij} , with adjacency matrices \mathbf{A}_{ij} , for $i \neq j$, are biregular, and the subgraphs G_{ii} are regular.

We finally recall that the *Kronecker product* of two matrices $\mathbf{A} = (a_{ij})$ and \mathbf{B} , denoted by $\mathbf{A} \otimes \mathbf{B}$, is obtained by replacing each entry a_{ij} with the matrix $a_{ij}\mathbf{B}$, for all i and j . Then, if \mathbf{u} and \mathbf{v} are eigenvectors of \mathbf{A} and \mathbf{B} , with corresponding eigenvalues λ and μ , respectively, then $\mathbf{u} \otimes \mathbf{v}$ (seeing \mathbf{u} and \mathbf{v} as matrices) is an eigenvector of $\mathbf{A} \otimes \mathbf{B}$, with eigenvalue $\lambda\mu$.

3 Three main results

The objective of this section is to obtain three general spectral upper bounds for α_k . Our first Theorem 3.1 is a very general bound. Since it depends on a certain polynomial $p \in \mathbb{R}_k[x]$, it is difficult to study when it is sharp in general, but it can be seen as a generalization of the previous Theorem 1.4. Our second Theorem 3.2 is a significant improvement to Theorem 1.5 and is sharp for some values of k , as shown using computer-assisted calculations. Finally, our last Theorem 3.7 provides an antipodal-like bound that generalizes Theorem 1.3.

Let G be a graph with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Let $[2, n] = \{2, 3, \dots, n\}$. Given a polynomial $p \in \mathbb{R}_k[x]$, we define the following parameters:

- $W(p) = \max_{u \in V} \{(p(\mathbf{A}))_{uu}\};$
- $w(p) = \min_{u \in V} \{(p(\mathbf{A}))_{uu}\};$
- $\Lambda(p) = \max_{i \in [2, n]} \{p(\lambda_i)\};$
- $\lambda(p) = \min_{i \in [2, n]} \{p(\lambda_i)\}.$

In the following three results, G is a graph with n vertices, adjacency matrix \mathbf{A} and eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Let $p \in \mathbb{R}_k[x]$ with corresponding parameters $W(p)$, $w(p)$, $\Lambda(p)$ and $\lambda(p)$.

3.1 A Cvetković-like bound

Theorem 3.1. *Let $p \in \mathbb{R}_k[x]$ with corresponding parameters $W(p)$, $w(p)$. Then, the k -independence number of G satisfies the bound*

$$\alpha_k \leq \min\{|\{i : p(\lambda_i) \geq w(p)\}|, |\{i : p(\lambda_i) \leq W(p)\}|\}.$$

Proof. We use the interlacing approach. Assume U is a k -independent set of G . We arrange the columns and rows of \mathbf{A} to have the vertices of U appearing in the first positions.

This implies that, for any polynomial $p(x)$ of degree at most k , the principal submatrix with the first $|U|$ rows and columns of $p(\mathbf{A})$ is diagonal. Call this matrix \mathbf{D} . Choosing $\mathbf{S}^T = \begin{pmatrix} \mathbf{I}_{|U|} & \mathbf{O} \end{pmatrix}$, we have

$$\mathbf{S}^T p(\mathbf{A}) \mathbf{S} = \mathbf{D}.$$

Let μ be the smallest eigenvalue of \mathbf{D} . From interlacing, it follows that there must be at least $|U|$ eigenvalues of $p(\mathbf{A})$ larger than μ . Noting that $w(p) \leq \mu$, we have $|U| \leq |\{i : p(\lambda_i) \geq w(p)\}|$. The other bound is proved analogously. \square

It is well known that Theorem 1.1 (Cvetkovic's bound) holds for weighted adjacency matrices. Thus, in our result above, instead of talking about polynomials of degree at most k , we could simply say "let \mathbf{M} be any matrix whose support consists of entries corresponding to vertices at distance at most k ...". The downside of this approach is that it is in general quite hard to find the optimal \mathbf{M} . Our approach in this work is interesting if one can come up with a good choice for the polynomial $p \in \mathbb{R}_k[x]$ or with an efficient method (like linear programming) to compute it in practice.

An analogous remark also applies to the next results, if one considers that the k -independence number of a graph G is precisely the independence number of the graph formed by making all pairs of vertices of G at distance at most k adjacent. For this graph, say $G^{(k)}$, one can formulate an optimization problem over completely positive matrices whose optimal value is equal to its independence number [17]. The semidefinite relaxation of this programming yields the Lovász Theta number of $G^{(k)}$, which upper bounds $\alpha_k(G)$. The spectral bounds we find below can all be obtained as the objective value of some feasible solution to the minimization formulation of the Lovász Theta semidefinite programming, therefore they are all larger or equal than the Lovász Theta number of $G^{(k)}$. We point out however that computing our spectral bounds is significantly faster than solving an SDP, and in many cases they perform fairly good, as we will point in some tables below.

3.2 A Hoffman-like bound

Theorem 3.2. *Let G be a regular graph with n vertices and eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. Let $p \in \mathbb{R}_k[x]$ with corresponding parameters $W(p)$ and $\lambda(p)$, and assume $p(\lambda_1) > \lambda(p)$. Then,*

$$\alpha_k \leq n \frac{W(p) - \lambda(p)}{p(\lambda_1) - \lambda(p)}. \quad (1)$$

Proof. Let \mathbf{A} be the adjacency matrix of G . Let U be a k -independent set of G with $r = |U| = \alpha_k(G)$ vertices. Again, assume the first columns (and rows) of \mathbf{A} correspond to the vertices in U . Consider the partition of said columns according to U and its complement. Let \mathbf{S} be the normalized characteristic matrix of this partition. The quotient

matrix of $p(\mathbf{A})$ with regards to this partition is given by

$$\mathbf{S}^T p(\mathbf{A}) \mathbf{S} = \mathbf{B}_k = \begin{pmatrix} \frac{\frac{1}{r} \sum_{u \in U} (p(\mathbf{A}))_{uu}}{rp(\lambda_1) - \sum_{u \in U} (p(\mathbf{A}))_{uu}} & p(\lambda_1) - \frac{\frac{1}{r} \sum_{u \in U} (p(\mathbf{A}))_{uu}}{rp(\lambda_1) - \sum_{u \in U} (p(\mathbf{A}))_{uu}} \\ p(\lambda_1) - \frac{\frac{1}{r} \sum_{u \in U} (p(\mathbf{A}))_{uu}}{rp(\lambda_1) - \sum_{u \in U} (p(\mathbf{A}))_{uu}} & p(\lambda_1) - \frac{\frac{1}{r} \sum_{u \in U} (p(\mathbf{A}))_{uu}}{rp(\lambda_1) - \sum_{u \in U} (p(\mathbf{A}))_{uu}} \end{pmatrix}, \quad (2)$$

with eigenvalues $\mu_1 = p(\lambda_1)$ and

$$\mu_2 = \text{tr } \mathbf{B}_k - p(\lambda_1) = \frac{1}{r} \sum_{u \in U} (p(\mathbf{A}))_{uu} - \frac{rp(\lambda_1) - \sum_{u \in U} (p(\mathbf{A}))_{uu}}{n - r}.$$

Then, by interlacing, we have

$$\lambda(p) \leq \mu_2 \leq W(p) - \frac{rp(\lambda_1) - rW(p)}{n - r}, \quad (3)$$

whence, solving for r and taking into account that $p(\lambda_1) - \lambda(p) > 0$, the result follows. \square

Let us now consider some particular cases of Theorem 3.2.

The case $k = 1$.

As mentioned above, α_1 coincides with the standard independence number. In this case we can take p as any linear polynomial satisfying $p(\lambda_1) > \lambda(p)$, say $p(x) = x$. Then, we have $W(p) = 0$, $p(\lambda_1) = \lambda_1$, $\lambda(p) = p(\lambda_n) = \lambda_n$, and (1) gives

$$\alpha_1 = \alpha \leq n \frac{-\lambda_n}{\lambda_1 - \lambda_n}, \quad (4)$$

which is Hoffman's bound in Theorem 1.2.

The case $k = 2$.

By making the right choice of a polynomial of degree two, we get the following result.

Corollary 3.3. *Let G be a δ -regular graph with n vertices, adjacency matrix \mathbf{A} , and distinct eigenvalues $\theta_0(= \delta) > \theta_1 > \dots > \theta_d$ with $d \geq 2$. Let θ_i be the largest eigenvalue such that $\theta_i \leq -1$. Then, the 2-independence number satisfies*

$$\alpha_2 \leq n \frac{\theta_0 + \theta_i \theta_{i-1}}{(\theta_0 - \theta_i)(\theta_0 - \theta_{i-1})}. \quad (5)$$

If the bound is attained, the matrix $\mathbf{A}^2 - (\theta_i + \theta_{i-1})\mathbf{A}$ has a regular partition (with a set of α_2 2-independent vertices and its complement) with quotient matrix

$$\mathbf{B} = \begin{pmatrix} \delta & \delta^2 - (\theta_i + \theta_{i-1} + 1)k \\ \delta + \theta_i \theta_{i-1} & \delta^2 - (\theta_i + \theta_{i-1} + 1)k - \theta_i \theta_{i-1} \end{pmatrix}. \quad (6)$$

Moreover, this is the best possible bound that can be obtained by choosing a polynomial and applying Theorem 3.2.

Proof. Note that only the last assertion is non-trivial, in view of Theorem 3.2. We now show why it holds. Let $p(x) = ax^2 + bx + c$ and suppose first that $a > 0$. Then, from the expression of the bound in (1), there is no loss of generality if we take $a = 1$ and $c = 0$. Then, the minimum of the polynomial $p(x) = x^2 + bx$ is attained at $x = -b/2$ and, hence, given b , the minimum $\lambda(p)$ must be equal to $p(\theta_i)$ where θ_i is the eigenvalue closest to $-b/2$. Now we proceed to find the optimal value for b . If $\theta_i \neq \theta_d$, from $(\theta_i + \theta_{i+1})/2 \leq -b/2 \leq (\theta_i + \theta_{i-1})/2$ we can write that $b = -\theta_i + \tau$ for $\tau \in [-\theta_{i-1}, -\theta_{i+1}]$. Otherwise, if $i = d$, from $-b/2 \leq (\theta_d + \theta_{d-1})/2$, we get that $b = -\theta_d + \tau$ with $\tau \geq -\theta_{d-1}$. Then, in both cases, with $W(p) = \theta_0$, $\lambda(p) = p(\theta_i) = \tau\theta_i$, and $p(\theta_0) = \theta_0^2 + (-\theta_i + \tau)\theta_0 (> \lambda(p))$, the bound in (1), as a function of τ , is

$$\Phi(\tau) = n \frac{\theta_0 - \theta_i \tau}{(\theta_0 - \theta_i)(\theta_0 + \tau)},$$

with derivative $\Phi'(\tau) = n \frac{-\theta_0(1+\theta_i)}{(\theta_0 - \theta_i)(\theta_0 + \tau)^2}$. Consequently, the resulting bound $\Phi(\tau)$ is an increasing, constant, or decreasing function depending on $\theta_i < -1$, $\theta_i = -1$, or $\theta_i > -1$, respectively. Since we are interested in the minimum value of Φ , we reason as follows:

- If $\theta_i < -1$, we must take the value of τ as small as possible, that is $\tau = -\theta_{i-1}$, which gives $\alpha_2 \leq \Phi(-\theta_{i-1}) = n \frac{\theta_0 + \theta_i \theta_{i-1}}{(\theta_0 - \theta_i)(\theta_i - \theta_{i-1})}$. Moreover, iterating the reasoning, we eventually take for θ_i the largest eigenvalue smaller than -1 , as claimed.
- If $\theta_i = -1$, we have that $\theta_{i+1} > -1$ and, with θ_i taking the role of θ_{i+1} , we are in the next case.
- If $\theta_i > -1$, we must take the value of τ as large as possible, that is $\tau = -\theta_{i+1}$, which gives $\alpha_2 \leq \Phi(-\theta_{i+1}) = n \frac{\theta_0 + \theta_i \theta_{i+1}}{(\theta_0 - \theta_i)(\theta_i - \theta_{i+1})}$. Again, iterating the procedure, we eventually take for θ_i the smallest eigenvalue greater than -1 , as claimed. Moreover, θ_{i+1} is the largest eigenvalue that is at most -1 , in agreement with our claim.

To show that our choice of the polynomial p is best possible, we assume now that $a < 0$ and, then, we reason with $p(x) = -x^2 + bx$. First, to satisfy the condition $p(\theta_0) > \lambda(p)$, we must have $b > \theta_0 + \theta_d$. Then, $\lambda(p) = p(\theta_d) = -\theta_d^2 - b\theta_d$ and the bound in (1) as a function of b , is

$$\Phi(b) = n \frac{-\theta_0 + \theta_d^2 - b\theta_d}{-\theta_0^2 + \theta_d^2 + b(\theta_0 - \theta_d)},$$

which is decreasing for $b > \theta_0 + \theta_d$. Then, we should take $\lim_{b \rightarrow \infty} \Phi(b) = n \frac{-\theta_d}{\theta_0 - \theta_d}$. But this is again the Hoffman's bound in (4) for α_1 , which is trivial for α_2 . Indeed, it is readily checked that, given n , θ_0 , and θ_{i-1} , the bound in (4) for α_1 is a decreasing function from $n/2$ (when $\theta_d = -\theta_0$) to $n/(\theta_0 + 1)$ (when $\theta_d = -1$); whereas the bound in (5) for α_2 is an increasing function from $n(1 - \theta_{i-1})/2(\theta_0 - \theta_{i-1})$ (when $\theta_i = -\theta_0$) to $n/(\theta_0 + 1)$ (when $\theta_i = -1$).

If equality in (5) holds, from (3) we conclude that $\mu_2 = \lambda(p)$ and, since $\mu_1 = p(\lambda_1)(= \Lambda(p))$, the interlacing is tight and the partition of $p(\mathbf{A})$ is regular. Finally, its quotient

matrix \mathbf{B} in (6) is obtained from (2) by using the right polynomial $p(x)$ and the bound of α_2 in (5). \square

Before giving some examples, we notice that the above choice of $\theta_i (\leq -1)$ always make sense because it is easy to prove (for example, using interlacing) that the smallest eigenvalue of a graph always satisfies this condition. In fact, as we have already seen (and one of the referees suggested to comment on), the bound in (5) attains its maximum value at $\theta_i = -1$, yielding $\alpha_2 \leq n/(k+1)$ for a k -regular graph G . Actually, this bound always holds and can be proved by using a simple combinatorial argument. Namely, as G is k -regular, the closed neighborhood of every vertex has cardinality $k+1$. Thus, in any 2-independent vertex set U , all these closed neighborhoods must be disjoint and, hence, $|U| \leq n/(k+1)$. Moreover, since for $\theta_i < 1$ the bound in (5) is strictly smaller than $n/(k+1)$, Corollary 3.3 can be viewed as a spectral generalization of this natural combinatorial bound. Of course, when the combinatorial bound is attained, G contains a 1-perfect code (with minimum codeword distance 3), in which case it is known that G has eigenvalue -1 (see, for instance, Godsil [15]).

In Table 1 we show the results of testing all named graphs from SAGE. The performance of our purely spectral bound from Corollary 3.3 (column denoted “Corollary 3.3”) is compared to the best bound that appears in [1] (column denoted “Bound [1]”), which, to our knowledge, is the best previously known bound for α_2 obtained via spectral methods only. Moreover, we compare the mentioned bounds to the values of the floor of the Lovász theta number of the distance at most 2 graph (column denoted “ ϑ_2 [20]”). The last column of the following table provides the actual value of α_2 . Regarding the last column, entries that say “time” denote that the computation took longer than 60 seconds on a standard laptop. The parameter α_k is computationally hard to determine, and it is not clear how long it would take to calculate the table entries that timed out. Note that in almost all cases our bound from Corollary 3.3 performs significantly better than the best previously known spectral bound in [1]. Also, it is worth noting that the bound $n/(k+1)$ outperforms the bound from [1] for all but the Heawood graph.

Apart from the examples in the table, we describe next two infinite families of (distance-regular) graphs where the bound of Corollary 3.3 is tight.

First, suppose that G is a connected *strongly regular* graph with parameters (n, k, a, c) (here we follow the notation of Godsil [15]). That is, G is a k -regular graph with n vertices, such that every pair of adjacent vertices have a common neighbours, and every pair of non-adjacent vertices have $c > 0$ common neighbours. Then, G has distinct eigenvalues

$$\theta_0 = k, \quad \theta_1 = \frac{1}{2}[a - c + \sqrt{(a - c)^2 + 4(a - c)}], \quad \theta_2 = \frac{1}{2}[a - c - \sqrt{(a - c)^2 + 4(a - c)}],$$

(for instance, see again [15]). Moreover, as $n = 1 + k + \frac{1}{c}[k(k - a + 1)]$, Corollary 3.3 gives $\alpha_2 = 1$, as it should be since G has diameter 2.

Now, let us take G an antipodal and bipartite distance-regular graph, with degree k and diameter 3. As shown in [4], these graphs have $n = 2(k+1)$ vertices, intersection

Name	Bound in [1]	ϑ_2 [20]	Corollary 3.3	α_2
Balaban 10-cage	32	17	17	17
Frucht graph	6	3	3	3
Meredith graph	20	10	14	10
Moebius-Kantor graph	8	4	4	4
Bidiakis cube	5	2	3	2
Gosset graph	2	2	2	2
Balaban 11-cage	41	26	27	time
Gray graph	33	11	11	11
Nauru graph	10	6	6	6
Blanusa first snark graph	8	4	4	4
Pappus graph	9	3	3	3
Blanusa second snark graph	8	4	4	4
Brinkmann graph	6	3	3	3
Harborth graph	24	10	10	10
Perkel graph	12	5	5	5
Harries graph	32	17	17	17
Bucky ball	23	12	14	12
Harries-Wong graph	32	17	17	17
Robertson graph	4	3	3	3
Heawood graph	2	2	2	2
Cell 600	18	8	8	8
Cell 120	302	120	120	120
Hoffman graph	6	2	2	2
Sylvester graph	8	6	6	6
Coxeter graph	13	7	7	7
Holt graph	10	3	4	3
Szekeres snark graph	25	10	12	9
Desargues graph	10	5	5	4
Horton graph	50	24	24	24
Dejter graph	44	16	16	16
Tietze graph	5	3	3	3
Double star snark	12	7	7	6
Truncated icosidodecahedron	60	28	30	26
Durer graph	5	2	2	2
Klein 3-regular Graph	22	13	13	12
Truncated tetrahedron	5	3	3	3
Dyck graph	14	8	8	8
Klein 7-regular graph	3	3	3	3
Tutte 12-cage	44	28	28	time
Ellingham-Horton 54-graph	32	12	13	11
Tutte-Coxeter graph	10	6	6	6
Ellingham-Horton 78-graph	38	19	19	18
Ljubljana graph	44	27	27	time
Tutte graph	21	10	11	10
F26A graph	12	6	6	6
Watkins snark graph	25	9	12	9
Flower snark	7	5	5	5
Markstroem graph	11	6	6	6
Wells graph	6	3	3	2
Folkman graph	10	3	3	3
Foster graph	44	22	22	21
McGee graph	10	5	6	5
Franklin graph	6	2	3	2
Hexahedron	2	2	2	2
Dodecahedron	9	4	4	4
Icosahedron	2	2	2	2

Table 1: Comparison between different bounds for the 2-independence number.

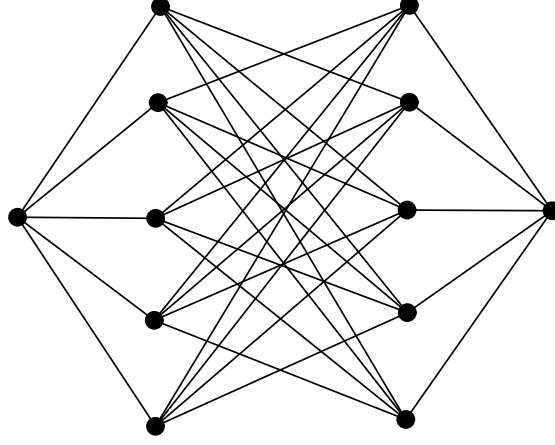


Figure 1: An antipodal and bipartite distance-regular graph with degree 5.

array $\{k, k-1, 1; 1, k-1, k\}$, and distinct eigenvalues

$$\theta_0 = k, \theta_1 = 1, \theta_2 = -1, \theta_3 = -k. \quad (7)$$

They are also uniquely determined for each k . They are the complement of the line graph of the complete bipartite graph $K_{2,k+1}$, denoted by $L(K_{2,k+1})$. Alternatively, G can be constructed from $K_{k+1,k+1}$ minus a perfect matching. In particular for $k = 2, 3$ we obtain the hexagon and the 3-cube, respectively. In Figure 1 we show the case of $k = 5$. With the eigenvalues in (7), Corollary 3.3 then gives $\alpha_2 \leq 2$, which is tight since the graph is 2-antipodal, as shown in the example of the figure. Moreover, since $\theta_1 + \theta_2 = 0$, the polynomial in Corollary 3.3 is just $p(x) = x^2$, and hence the matrix \mathbf{A}^2 has a regular partition with the following quotient matrix given by (6):

$$\mathbf{B} = \begin{pmatrix} k & k(k-1) \\ k-1 & k(k-1)+1 \end{pmatrix}. \quad (8)$$

The case of general k .

Another consequence of Theorem 3.2 is the subsequent Corollary 3.5, which is closely related to Theorem 1.5. This is due to the fact that both results make use of the same polynomial $p(x) = x + x^2 + \cdots + x^k$, although the bounds given in Corollary 3.5 constitute a significant improvement. Before proving them, we give the following result, which is equivalent to Theorem 3.2, in the sense that the minimization of the ratio over all polynomials satisfying the hypotheses will yield to the same bound.

Corollary 3.4. *Let G be a regular graph with n vertices and eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. Let $p \in \mathbb{R}_k[x]$ with corresponding parameter $W(p)$, satisfying $p(\lambda_i) \geq 0$ for all $i = 2, \dots, n$. Then,*

$$\alpha_k \leq n \frac{W(p)}{p(\lambda_1)}. \quad (9)$$

Proof. Assume that the polynomial q with $q(\lambda_1) > \lambda(q)$ gives the best bound in Theorem 3.2. Then, for any constant c , the result does not change if we replace q by $q + c$ (since $W(p+c) = W(p) + c$, $\lambda(q+c) = \lambda(q) + c$, and $(p+c)(\lambda_1) = p(\lambda_1) + c$). In particular, taking $c = \lambda(q)$, the polynomial $p(x) = q(x) - \lambda(q)$, satisfies $p(\lambda_i) \geq 0$ for all i , and $\lambda(p) = 0$. Thus, (1) becomes (9). Moreover, let us see that here we do not need the assumption $p(\lambda_1) > \lambda(p)$. Indeed, first note that, for any polynomial p , if $W(p) \geq p(\lambda_1)$, then both bounds, (1) and (9), are trivial. Thus, we can assume that $p(\lambda_1) > W(p)$. Then,

$$np(\lambda_1) > nW(p) \geq \text{tr } p(\mathbf{A}) = \sum_{i=1}^n p(\lambda_i) \geq p(\lambda_1) + (n-1)\lambda(p),$$

so that $p(\lambda_1) > \lambda(p)$. □

If $\nu = \max\{|\lambda_2|, |\lambda_n|\}$, and upon choosing $p(x) = \sum_{\ell=1}^k x^\ell + \sum_{\ell=1}^k \nu^\ell$, it is easy to see that $p(\lambda_i) \geq 0$ for all i , and that the previous corollary gives precisely Theorem 1.5. We can do better using the same polynomial, noting that $\lambda(p)$ can be computed explicitly for the case when k is odd, and a reasonable lower bound for it can be found for when k is even.

Corollary 3.5. *Let G be a δ -regular graph with n vertices and distinct eigenvalues $\theta_0(= \delta) > \theta_1 > \dots > \theta_d$. Let $W_k = W(p) = \max_{u \in V} \{\sum_{i=1}^k (\mathbf{A}^k)_{uu}\}$. Then, the k -independence number of G satisfies the following:*

(i) *If k is odd, then*

$$\alpha_k \leq n \frac{W_k - \sum_{j=0}^k \theta_d^j}{\sum_{j=0}^k \delta^j - \sum_{j=0}^k \theta_d^j}. \quad (10)$$

(ii) *If k is even, then*

$$\alpha_k \leq n \frac{W_k + 1/2}{\sum_{j=0}^k \delta^j + 1/2}. \quad (11)$$

Proof. For odd k , the polynomial $p(x) = x + x^2 + \dots + x^k$ is strictly increasing for any x . This can be seen, for instance, realizing that its derivative, for odd $k > 3$, can be written as

$$\frac{d}{dx} p(x) = \sum_{j=1}^{(k-1)/2} j(x^{j-1} + x^j)^2 + \frac{k+1}{2} x^{k-1},$$

which is a sum of only non-negative terms. Thus the (negative) value of $\lambda(p)$ is always $\sum_{j=0}^k \theta_d^j$, and Theorem 3.2 gives the desired bound in (i).

For even k , note that $p(x) \geq -(1/2)$ for all x , as in fact,

$$p(x) + 1/2 = \frac{1}{2} \sum_{j=1}^{k/2} (x^{j-1} + x^j)^2 + \frac{1}{2} x^k$$

Therefore (ii) follows from Corollary 3.4 applied to $p(x) + 1/2$. We leave it to the reader to verify that $1/2$ is the best constant we can use as, for even k , the minimum of $p(x)$ approaches $-1/2$ as k grows. \square

The case of walk-regularity.

Assume now that G is *walk-regular*, that is, for any fixed $k \geq 0$, the number $a_{uu}^{(k)}$ of closed walks of length k rooted at a vertex u does not depend on u . As a consequence, for any polynomial $p(x)$, $W(p) = \frac{1}{n} \text{tr } p(\mathbf{A})$.

Corollary 3.6. *Let $G = (V, E)$ be a walk-regular graph, with degree δ , n vertices, and spectrum $\text{sp } G = \{\theta_0 (= \delta), \theta_1^{m_1}, \dots, \theta_d^{m_d}\}$, where $\theta_0 > \dots > \theta_d$. Let $p = q_k$ be the sum polynomial $q_k = p_0 + \dots + p_k$, for $k = 0, \dots, d-1$, where the p_i 's stand for the predistance polynomials of G . Then, for $k = 1, \dots, d-1$, the k -independence number of G satisfies*

$$\alpha_k(G) \leq n \frac{1 - \lambda(q_k)}{q_k(\delta) - \lambda(q_k)}.$$

Proof. Notice that, since G is walk-regular, $(\mathbf{A}^\ell)_{uu} = \frac{1}{n} \text{tr } \mathbf{A}^\ell$ for any $u \in V$ and $\ell = 0, 1, \dots, k$. Thus,

$$W(q_k) = \frac{1}{n} \text{tr } q_k(\mathbf{A}) = \frac{1}{n} \sum_{i=0}^d m_i q_k(\theta_i) = \langle q_k, 1 \rangle_G = \|p_0\|^2 = 1,$$

where we used that $p_0 = 1$. Moreover, from the orthogonality of the polynomials q_i 's, $q_0 = 1$, and every $k = 1, \dots, d-1$, we have

$$\langle 1, q_k \rangle_{[G]} = \frac{1}{n} \sum_{i=1}^d m_i (\theta_0 - \theta_i) q_k(\theta_i) = 0.$$

Thus, since $m_i(\theta_0 - \theta_i) > 0$, it must be $q_k(\theta_i) \leq 0$ for some $i > 0$. Hence, as $q_k(\theta_0) > 0$, we have $q_k(\theta_0) > \lambda(q_k)$, as required. Then, the result follows from Theorem 3.2. \square

k	3	4	5	6	7
$P_k(\theta_0)$ ($\theta_0 = \delta = 49$)	1115/81	485/9	8629/25	3431	–
W_k ($p = x + \dots + x^k$)	637	17150	469910	15193479	537790827
$\lambda(p)$ ($p = x + \dots + x^k$)	-301	0	-14707	0	-720601
$q_k(\delta)$	1716	2941	3382	3431	3432
$\lambda(q_k)$	-40	-75	-24	-1	0
Bound from Theorem 1.3	464	125	20	2	–
Bound from Theorem 1.5	935	721	546	408	302
Bound from Corollary 3.5	26	10	5	3	2
Bound from Corollary 3.6	80	86	25	2	1

Table 2: Comparison of bounds for α_k in the Johnson graph $J(14, 7)$.

An Example

To compare the above bounds with those obtained in [8] and [1] (here in Theorems 1.3 and 1.5, respectively), let us consider G to be the Johnson graph $J(14, 7)$ (see, for instance, [4, 15]). This is an antipodal (but not bipartite) distance-regular graph, with $n = 3432$ vertices, diameter $D = 7$, and spectrum

$$\text{sp } G = \{49^1, 35^{13}, 23^{77}, 13^{273}, 5^{637}, -1^{1001}, -5^{1001}, -7^{429}\}.$$

In Table 2 we show the bounds obtained for α_k , together with the values of $P_k(\theta_0)$, W_k , $\lambda(p)$, $q_k(\delta)$, and $\lambda(q_k)$, for $k = 3, \dots, 7$. Since every distance-regular graph is also walk-regular, the value of W_k is just $\frac{1}{n} \text{tr } p(\mathbf{A})$, easily computed from the spectrum. Note that, in general, the bounds obtained by the above corollaries constitute a significant improvement with respect to those in [8, 1]. In particular, the bounds for $k = 6, 7$ are either equal or quite closed to the correct values $\alpha_6 = 2$ (since G is 2-antipodal, and $\alpha_7 = 1$ (since $D = 7$)).

As suggested by one of the referees, some of these bounds for α_k can be further improved (or reobtained) if we apply Corollary 3.3 to the distance at most $k/2$ graph of G . For instance, the distance 1-or-2 graph of $G = J(14, 7)$, usually denoted by $G_1 \cup G_2$, has eigenvalues 490, 224, 74, 14, 4, -10 , -16 . Then, Corollary 3.3 yields $\alpha_4 \leq 6$, which is a better bound than any given in Table 2. Similarly, using the distance at most 3 of $J(14, 7)$, we get again the correct bound of 2 for α_6 .

3.3 An antipodal-like bound

Theorem 3.7. *Let G be a regular graph with a maximum k -independent set of size r . Let $p \in \mathbb{R}_k[x]$ be a polynomial satisfying $p(\lambda_1) \geq \Lambda(p) > 0$, $\lambda(p) < 0$, and assume that $\Lambda(p) \geq |\lambda(p)|(r - 1)$. Then,*

$$r = \alpha_k \leq 1 + \frac{\Lambda(p)}{p(\lambda_1)}(n - 1). \quad (12)$$

Proof. Let $U = \{u_0, u_1, \dots, u_{r-1}\}$ be a maximum k -independent set, where $r = |U| = \alpha_k$. The matrix $p(\mathbf{A})$ has eigenvalues $p(\lambda_1) \geq \Lambda(p)$ and $p(\lambda_i)$ satisfying $\lambda(p) \leq p(\lambda_i) \leq \Lambda(p)$ for $2 \leq i \leq n$. Now consider the matrix $\mathbf{B} := \mathbf{A}(K_r) \otimes p(\mathbf{A})$. For instance, for $r = 3$ we have

$$\mathbf{B} = \left(\begin{array}{c|c|c} \mathbf{O} & p(\mathbf{A}) & p(\mathbf{A}) \\ \hline p(\mathbf{A}) & \mathbf{O} & p(\mathbf{A}) \\ \hline p(\mathbf{A}) & p(\mathbf{A}) & \mathbf{O} \end{array} \right).$$

The complete graph K_r has eigenvalues $r - 1$, and -1 with multiplicity $r - 1$, with corresponding orthogonal eigenvectors $\phi_0 = \mathbf{j} \in \mathbb{R}^r$ and $\phi_i = (1, \omega^i, \omega^{2i}, \dots, \omega^{(r-1)i})^\top$, $1 \leq i \leq r - 1$, where ω is a primitive r -th root of unity, say $\omega := e^{j\frac{2\pi}{r}}$. Consequently, each eigenvector \mathbf{u} of $p(\mathbf{A})$, with eigenvalue $p(\lambda)$, $\lambda \in \text{sp } G$, gives rise to the eigenvalues $(r - 1)p(\lambda)$, and $-p(\lambda)$ with multiplicity $r - 1$, with corresponding orthogonal eigenvectors $\mathbf{u}_0 := \mathbf{j} \otimes \mathbf{u}$ and $\mathbf{u}_i := \phi_i \otimes \mathbf{u}$, $1 \leq i \leq r - 1$. Thus, when $\lambda \neq \lambda_1$, we know that $\lambda(p) \leq p(\lambda) \leq \Lambda(p)$ and, hence, the corresponding eigenvalues of \mathbf{B} are within the interval $[\lambda(p)(r - 1), \Lambda(p)(r - 1)]$. Moreover, \mathbf{B} has maximum eigenvalue $(r - 1)p(\lambda_1) \geq \Lambda(p)(r - 1)$.

Now consider the (column) vector $\mathbf{f}_U := (e_{u_0}^\top | e_{u_1}^\top | \dots | e_{u_{r-1}}^\top)^\top \in \mathbb{R}^{rn}$, and consider its spectral decomposition:

$$\mathbf{f}_U = \sum_{i=0}^{r-1} \frac{\langle \mathbf{f}_U, \mathbf{j}_i \rangle}{\|\mathbf{j}_i\|^2} \mathbf{j}_i + \mathbf{z}_U = \frac{1}{n} \mathbf{j}_0 + \mathbf{z}_U \quad (13)$$

where $\mathbf{j}_i = \phi_i \otimes \mathbf{j}$, $\mathbf{z}_U \in \langle \mathbf{j}_0, \mathbf{j}_1, \dots, \mathbf{j}_{r-1} \rangle^\perp$, and we have used that $\langle \mathbf{f}_U, \mathbf{j}_0 \rangle = r$, $\|\mathbf{j}_0\|^2 = rn$, and $\langle \mathbf{f}_U, \mathbf{j}_i \rangle = \sum_{j=0}^{r-1} \omega^{ij} = 0$, for any $1 \leq i \leq r - 1$. From (13), we get

$$\|\mathbf{z}_U\|^2 = \|\mathbf{f}_U\|^2 - \frac{1}{n^2} \|\mathbf{j}_0\|^2 = r \left(1 - \frac{1}{n} \right).$$

Since there is no path of length $\leq k$ between any pair of vertices of U , $(p(\mathbf{A}))_{u_i u_j} = 0$ for any $i \neq j$. Thus,

$$\begin{aligned} 0 &= \langle \mathbf{B} \mathbf{f}_U, \mathbf{f}_U \rangle = \left\langle \frac{(r - 1)p(\lambda_1)}{n} \mathbf{j}_0 + \mathbf{B} \mathbf{z}_U, \frac{1}{n} \mathbf{j}_0 + \mathbf{z}_U \right\rangle \\ &= \frac{r(r - 1)p(\lambda_1)}{n} + \langle \mathbf{B} \mathbf{z}_U, \mathbf{z}_U \rangle \\ &\geq \frac{r(r - 1)p(\lambda_1)}{n} + (r - 1)\lambda(p)\|\mathbf{z}_U\|^2 \\ &= \frac{r(r - 1)}{n} p(\lambda_1) + (r - 1)\lambda(p)r \left(\frac{n - 1}{n} \right). \end{aligned}$$

Therefore, we get

$$p(\lambda_1) \leq -\lambda(p)(n - 1) = |\lambda(p)|(n - 1) \leq \frac{\Lambda(p)}{r - 1}(n - 1),$$

whence (12) follows. \square

As a consequence of the above theorem, we have the following result.

Corollary 3.8. *Let G be a regular graph with a maximum k -independent set of size α_k . Let $P \in \mathbb{R}_k[x]$ satisfying $P(\lambda_1) \geq \Lambda(P)$. Then,*

$$\alpha_k \leq \frac{n(\Lambda(P) - \lambda(P))}{P(\lambda_1) - \lambda(P)}. \quad (14)$$

Proof. Notice that, if $P \in \mathbb{R}_k[x]$ is a polynomial with $P(\lambda_1) \geq \Lambda(P)$, and $r > 1$, then the polynomial

$$p(x) = \frac{r}{\Lambda(P) - \lambda(P)} P(x) - \frac{r\lambda(P)}{\Lambda(P) - \lambda(P)} - 1$$

satisfies the hypotheses of Theorem 3.7. Then, using $p(x)$ with $r = \alpha_k$ in (12) and solving for α_k we obtain the desired result. \square

Note that if $P = P_k$, the k -alternating polynomial, Corollary 3.8 yields Theorem 1.3. In particular, in [8] it was shown that the bound (14) for α_{d-1} and $P = P_{d-1}$ is attained for every r -antipodal distance-regular graph with $d + 1$ distinct eigenvalues (see [8]). For example, one can easily check that, with the order and eigenvalues of $L(K_{2,k+1})$ in (7), the bound in Theorem 1.3 gives the right value $\alpha_2 = 2$.

4 Bounding the diameter

As a by-product of our results, we can also obtain upper bounds for the diameter of a graph G . This is because if $\alpha_k = 1$ for some k , then the diameter of G must satisfy $D \leq k$. To assure that $\alpha_k = 1$, we only need to obtain an upper bound smaller than 2. As an example, the following result follows as a direct consequence of Corollary 3.3.

Proposition 4.1. *Let G be a regular graph on n vertices, and with distinct eigenvalues $\theta_0 > \dots > \theta_d$, $d \geq 2$. Let θ_i the largest eigenvalue not greater than -1 . Then, if*

$$n \frac{\theta_0 + \theta_i \theta_{i-1}}{(\theta_0 - \theta_i)(\theta_0 - \theta_{i-1})} < 2$$

then G has diameter $D = 2$.

Another interesting conclusion is a result which was first obtained in [11]. Here we show it as a consequence of Corollary 3.8 by taking $P = P_k$, the k -alternating polynomial (that is, Theorem 1.3).

Proposition 4.2 ([11]). *Let G be a regular graph with n vertices, diameter D , and distinct eigenvalues $\theta_0 > \dots > \theta_d$. For some $k \leq d - 1$, let P_k be the corresponding k -alternating polynomial. If $P_k(\theta_0) > n - 1$, then $D \leq k$.*

Proof. The sufficient condition comes from assuming that $\alpha_k \leq \frac{2n}{P_k(\theta_0)+1} < 2$. □

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